updates on impurity density predictions and PT_SOLVER speedup

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Impurity density prediction

1): solve impurity element density equation

$$\frac{\partial}{\partial t}\left(V' n_z\right)+\frac{\partial}{\partial \rho}\left[V'\left\langle\left|\nabla\rho\right|^2\right\rangle\left(n_z v - D\nabla n_z\right)\right]-\zeta\frac{\partial}{\partial\rho}\left(\rho V' n_z\right)=s_z$$

(where v is pinch velocity, and D is total particle diffusivity from TGLF and NEO, can be combined with electron & ion temperature, electron density, angular momentum prediction.)

2): corona equilibrium equation for the density at each charge state

$$\frac{n_z^{i+1}}{n_z^{i}}=\frac{I_z^{i\to i+1}}{R_z^{i+1\to i}}$$

where $I_z^{i\to i+1}$ is the total ionization rate, and $R_z^{i+1\to i}$ is total recombination rate that are calculated based on ADAS data

3): ADAS data to predicate impurity radiation power loss

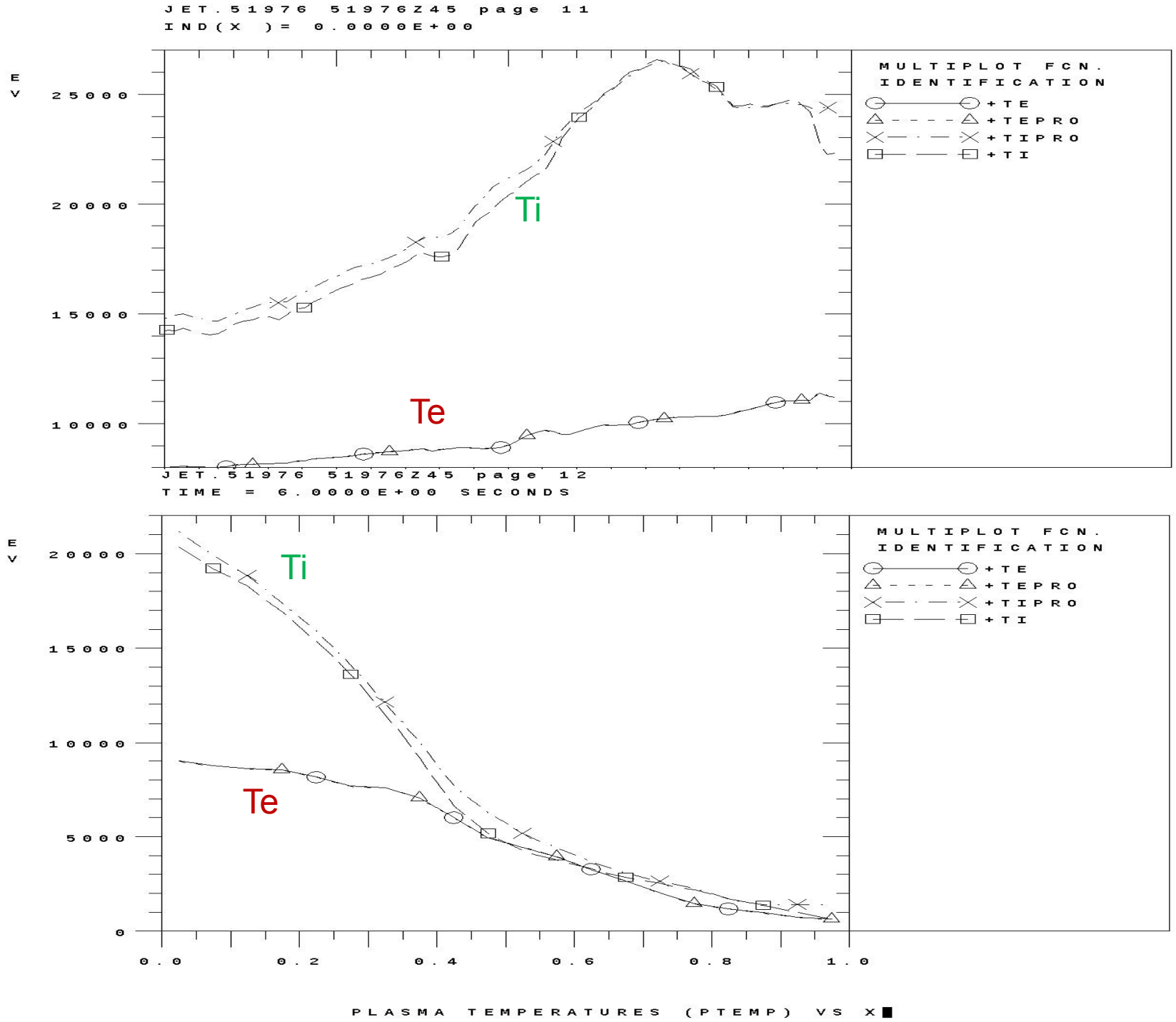
$$P_{rad}=\sum_i\left(\left\langle v\sigma\right\rangle_{line}+\left\langle v\sigma\right\rangle_{recomb}+\left\langle v\sigma\right\rangle_{brem}\right)n_z^i n_e$$

where line, recomb, and brem stands for line radiation, recombination, and bremsstrahlung-cascade power loss coefficients based on ADAS database.

usage and namelist setup

```
! PLASMA COMPOSITION:
AIMPS= 9.02, 12.01, 20.18, 58.69       !Be, C, Ne, Ni
XZIMPS=4.0, 6.0,10.0,28.0
NPRAD=2            ! to predict radiation
NADVSIM=1,1,1,1
NRADSIM=1       ! to use adas data
NADAS=1,1,1,1   ! to use adas data

! ADAS Be data
ADAS_YEAR(1,1) = 89   ! acd file
ADAS_YEAR(2,1) = 93   ! scd file
ADAS_YEAR(4,1) = 89   ! plt file
ADAS_YEAR(7,1) = 89   ! prb file

! ADAS C data
ADAS_YEAR(1,2) = 89   ! acd file
ADAS_YEAR(2,2) = 93   ! scd file
ADAS_YEAR(4,2) = 89   ! plt file
ADAS_YEAR(7,2) = 89   ! prb file

! ADAS Ne data
! ADAS Ni data
```

```
! PT_SOLVER for prediction
LPREDICTIVE_MODE=3
 ! choose predictive model
LPREDICT_TE=1
LPREDICT_TI=1
LPREDICT_PPHI=0
LPREDICT_NE=0
LPREDICT_NMAIN=0
LPREDICT_NIMP=1     ! to predict impurity density

 ! turbulent model selected
TR_TURB_AXIAL='NONE'
TR_NC_AXIAL='NONE'
TR_EXB_AXIAL='NONE'

TR_TURB_EDGE='NONE'
TR_NC_EDGE='NONE'
TR_EXB_EDGE='NONE'

TR_TURB_CONF='TGLF'          ! to use TGLF
TR_NC_CONF='NEOGK'           ! to use NEO
TR_EXB_CONF='DMEXB'
```



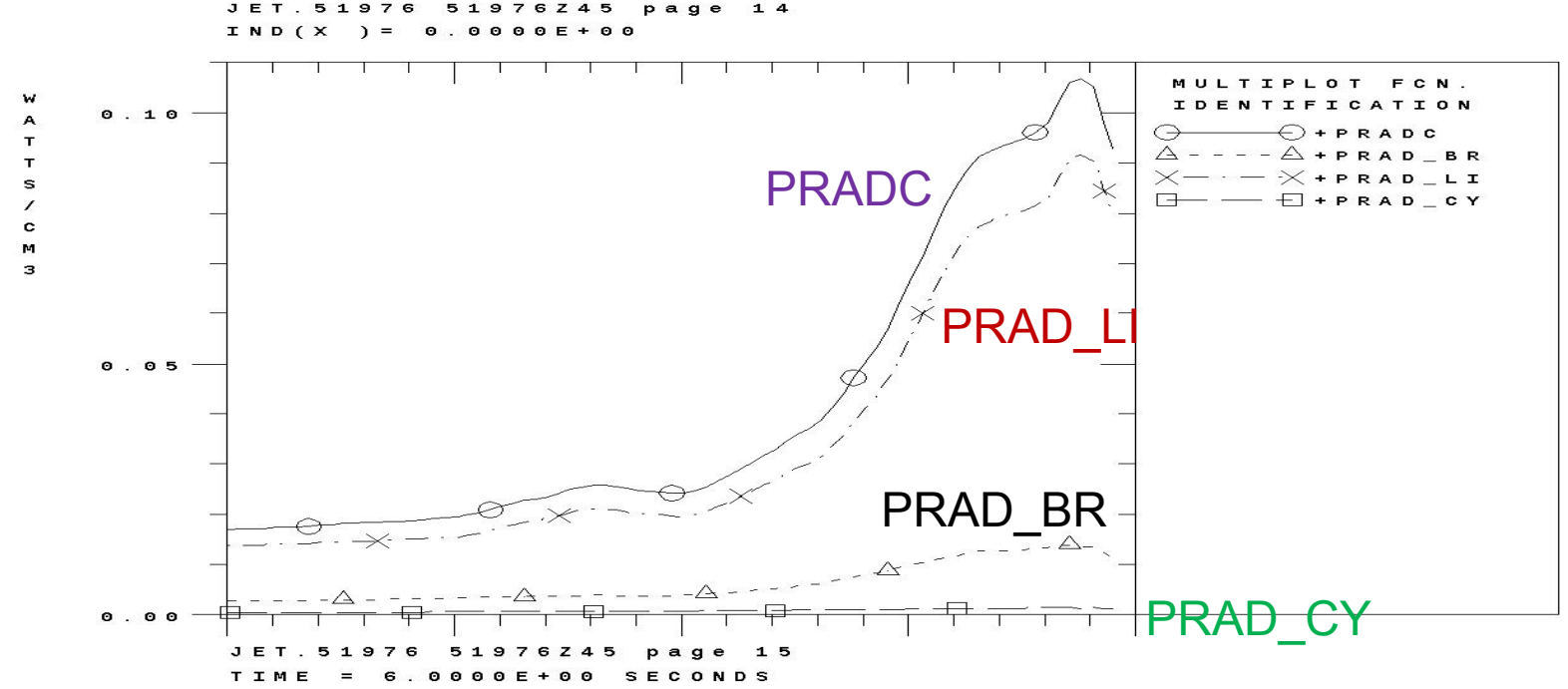
Test case

JET_51976 with total 6 species, 4 impurities (Be, C, Ne, Ni)

ADAS database is used to predict impurity radiation power loss

electron and ion temperatures are taken from user input ufiles

ADAS ionization and recombination rates are used to calculate the individual density profiles for different charge states



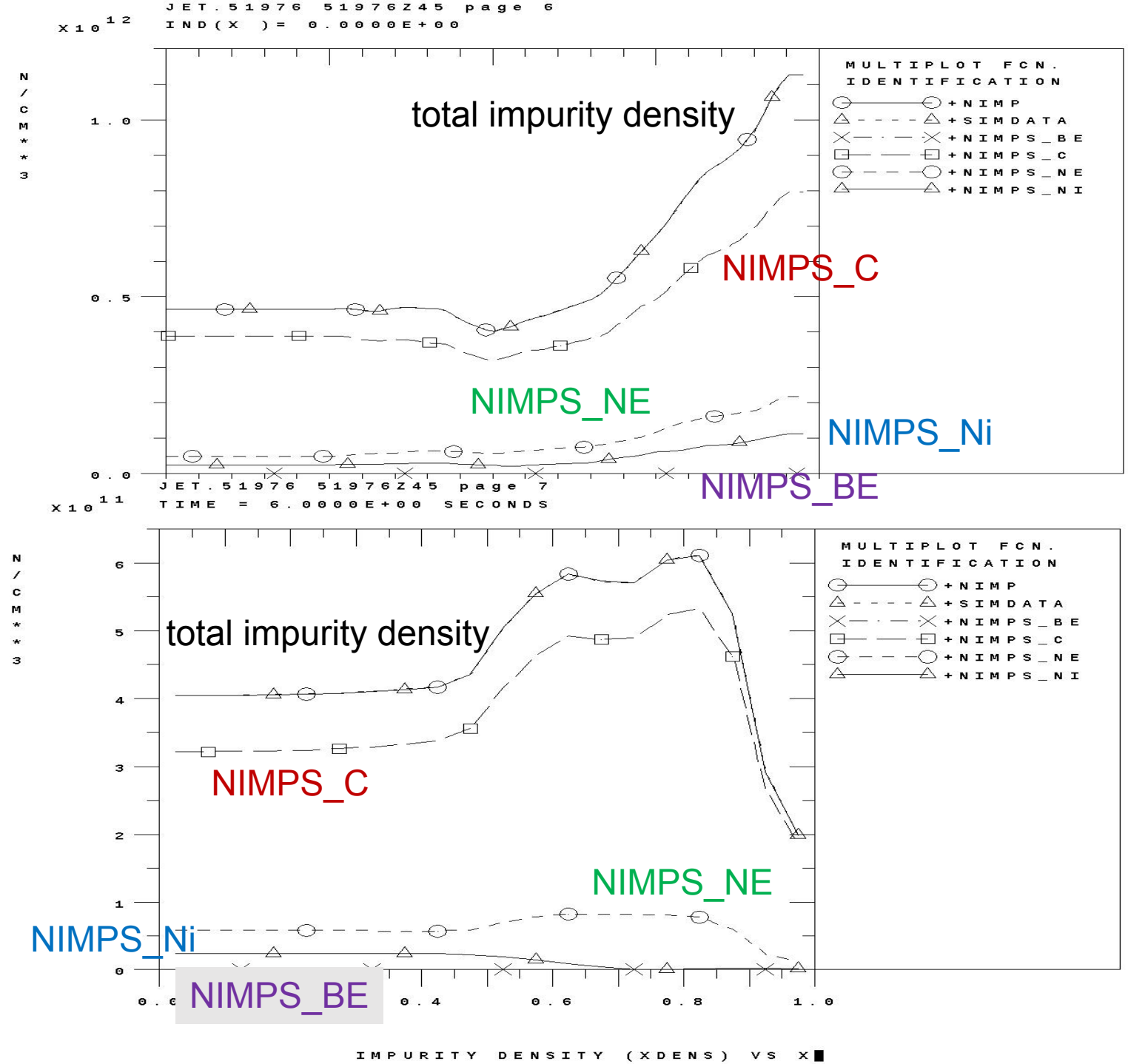
Test case

where PRAD_BR is total bremsstrahlung-cascade radiation power loss

PRAD_LI is total line radiation power loss

PRAD_CY is total total recombination radiation power loss.

PRADC is the total predicted radiation power loss



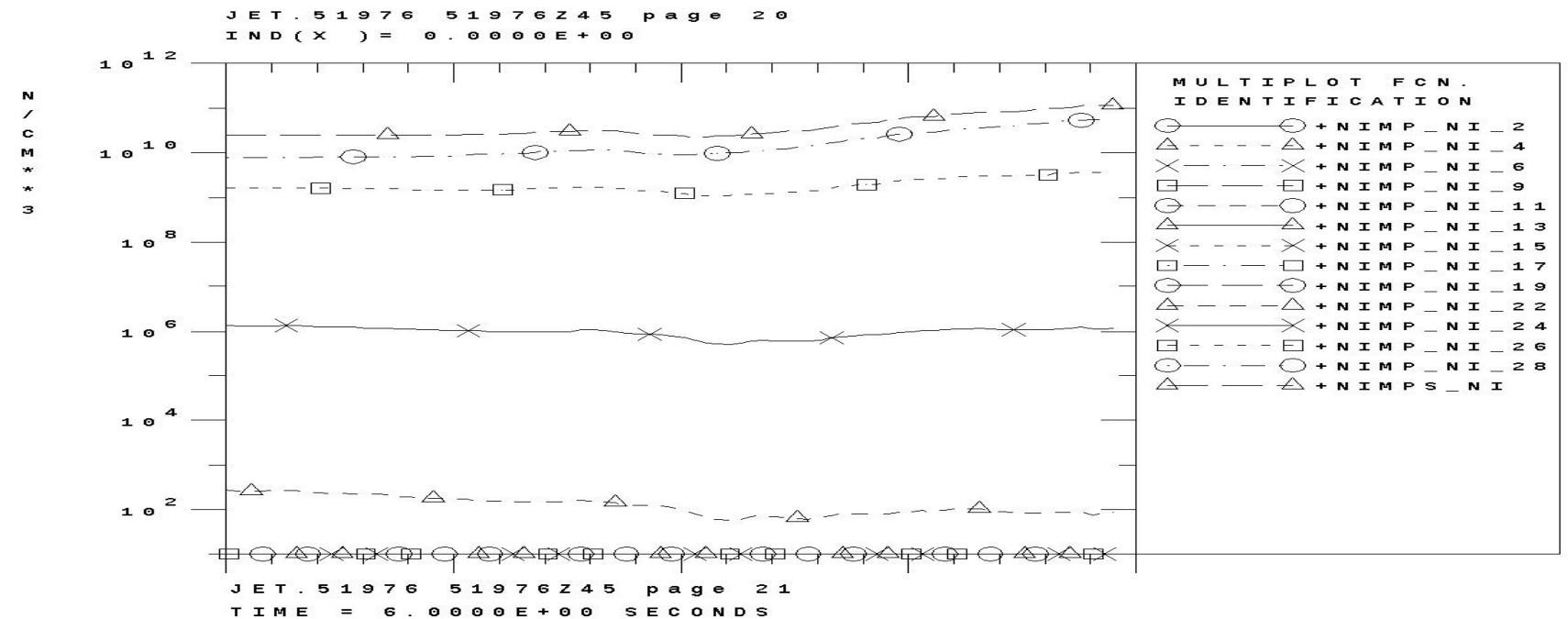
Test case

where NIMPS_BE is total Be impurity density

NIMPS_C is total Carbon impurity density

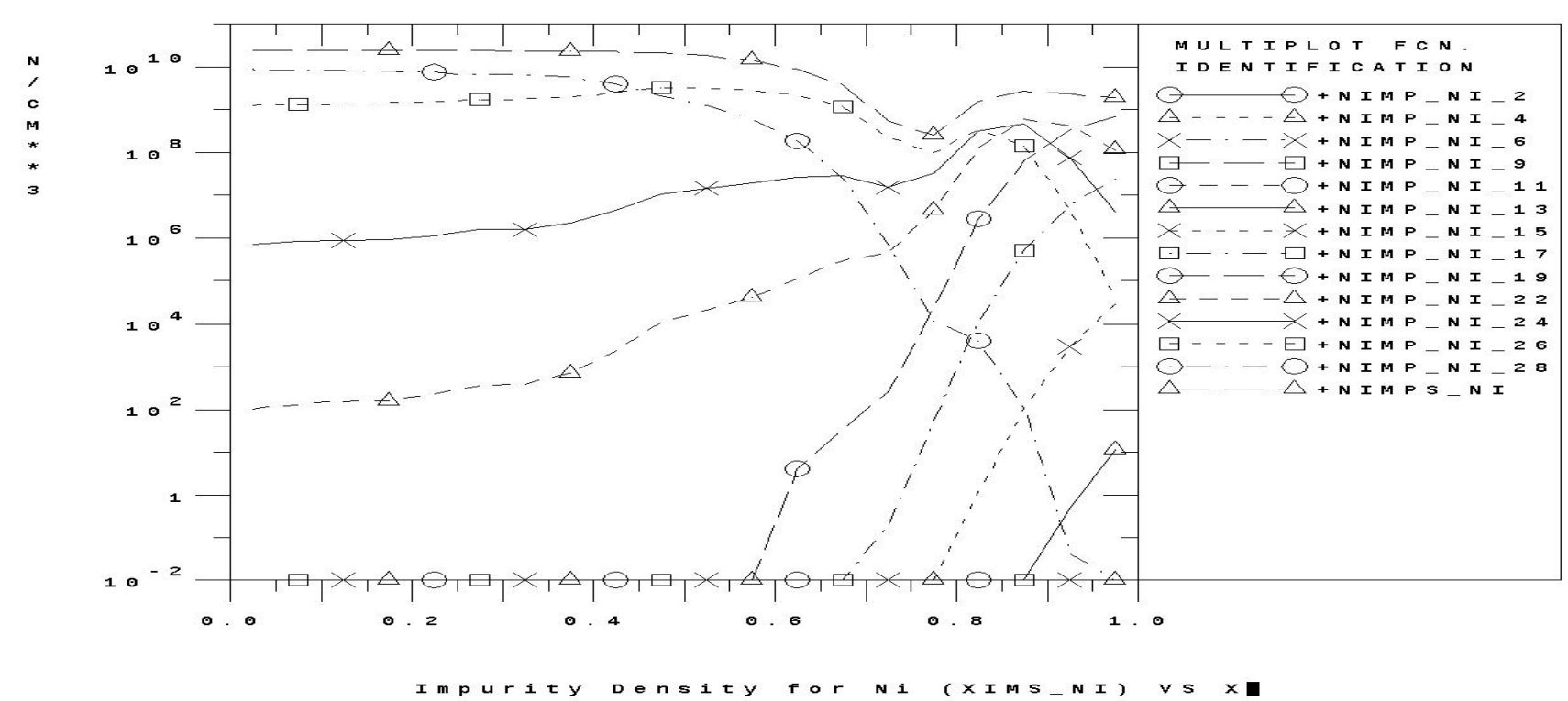
NIMPS_NE is total Ne impurity density.

NIMPS_Ni is the total Ni impurity density



Test case

Time history of Ni impurity density for individual charge states



Time evolution of Ni impurity density Profiles for individual charge states.

Interpolated differential operator (IDO) scheme

1): Interpolated differential operator (IDO) scheme solves the paricle, energy, and momentum conservation equations, and their derivative equations at the same time.

2): High order difference terms are calculated by using 3rd spline reconstruction, and 4th-order compact scheme.

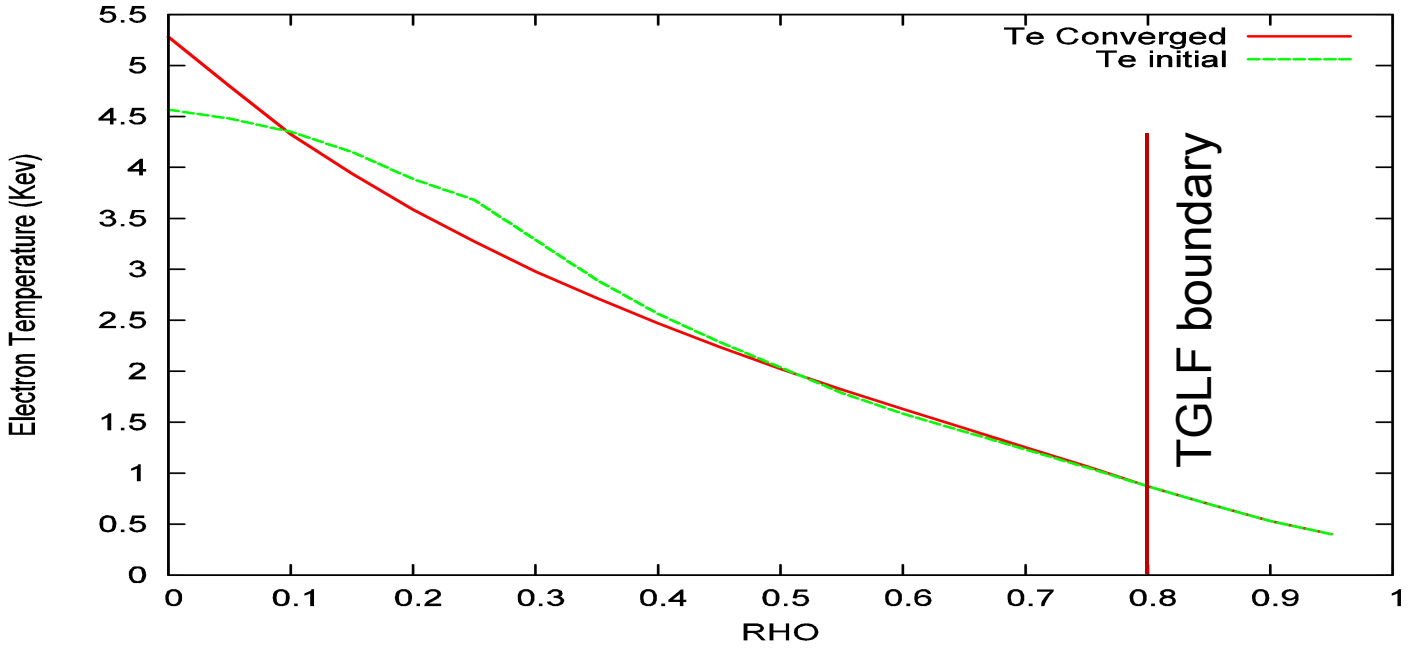
3): Newton iteration method is used to reach convergent solution

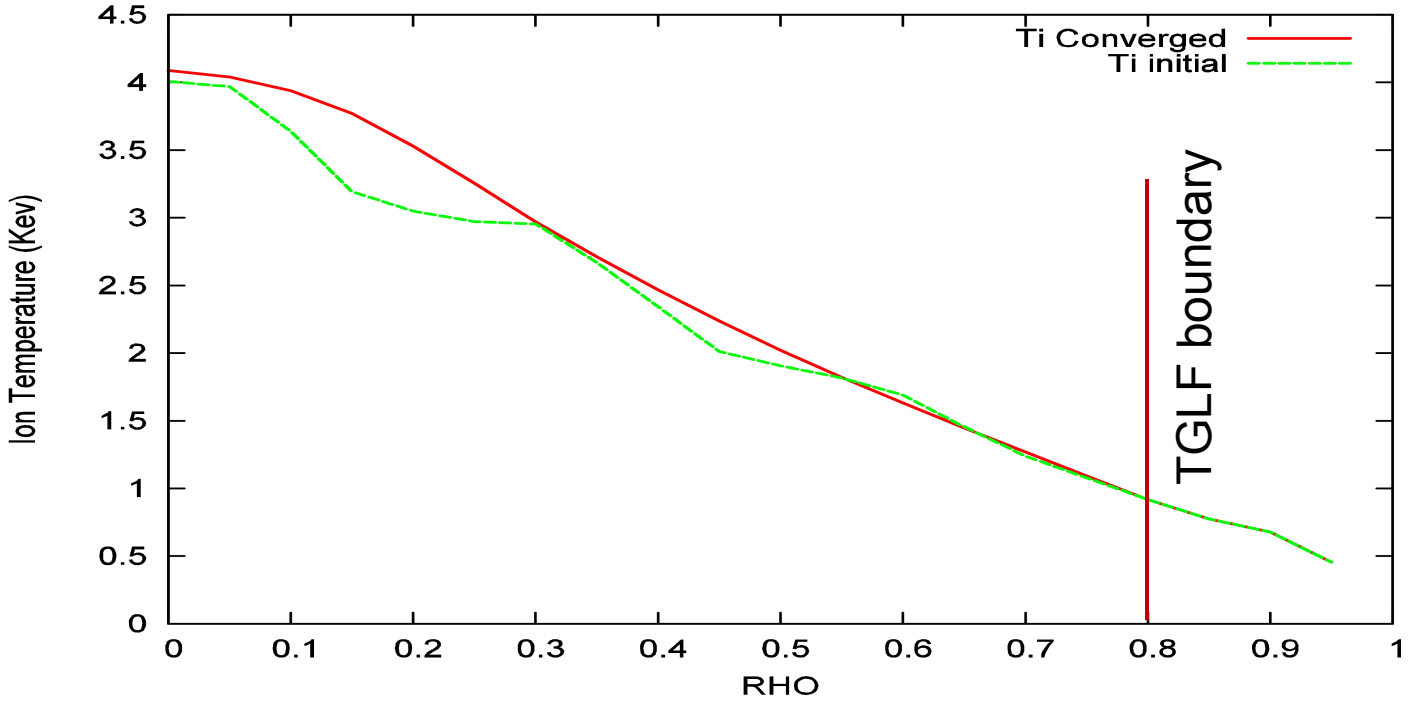
4): Over relaxation factor is applied to transport coefficients.

5): No additional numerical diffusivity required.

6): Large timestep

7): IDO scheme has been tested in FASTRAN code.



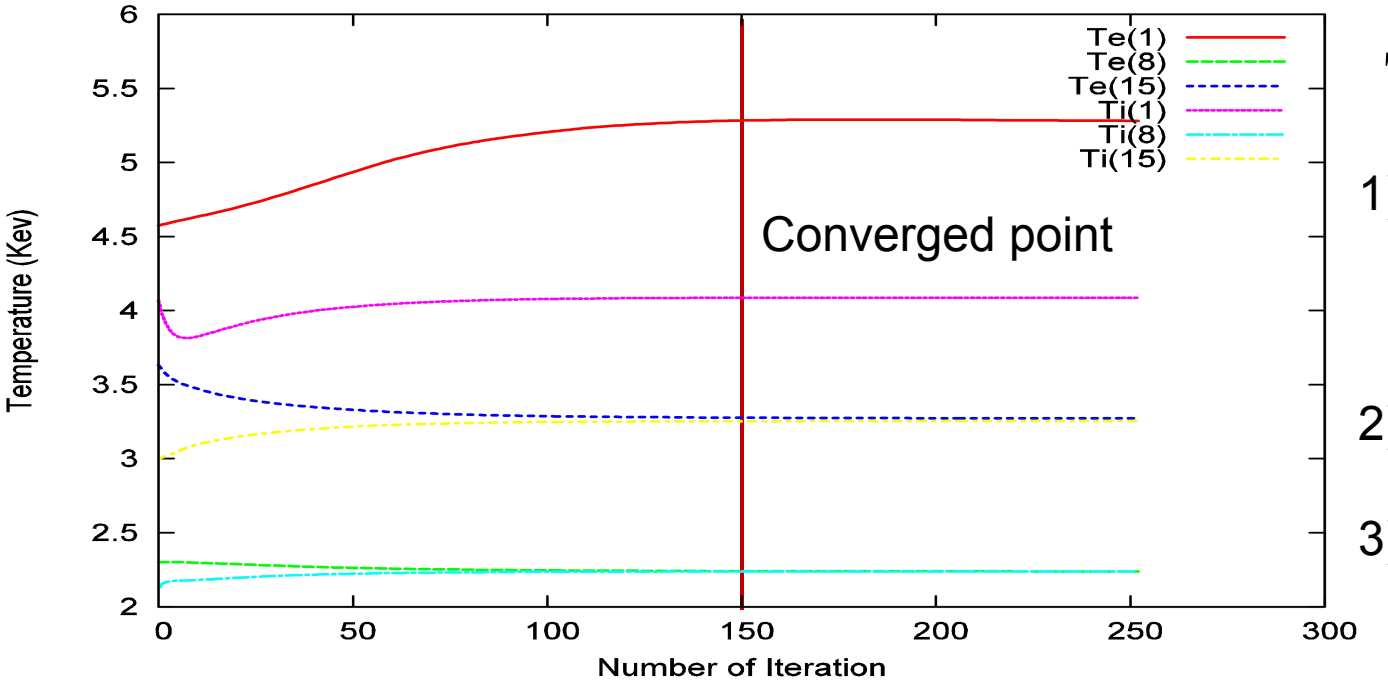


Test case

1): TFTR 88615 test case using TGLF and Chang-Hilton,

2): PT_SOLVER with IDO scheme to predict Te&Ti

3): Good agreement with experimental data (Te&Ti initial/exp)

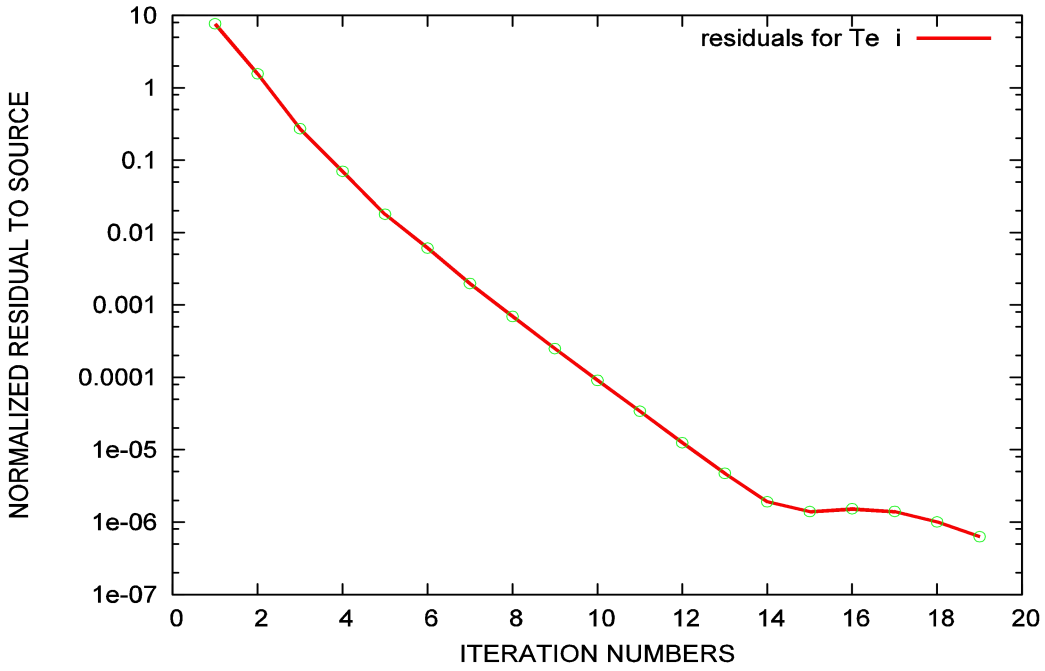


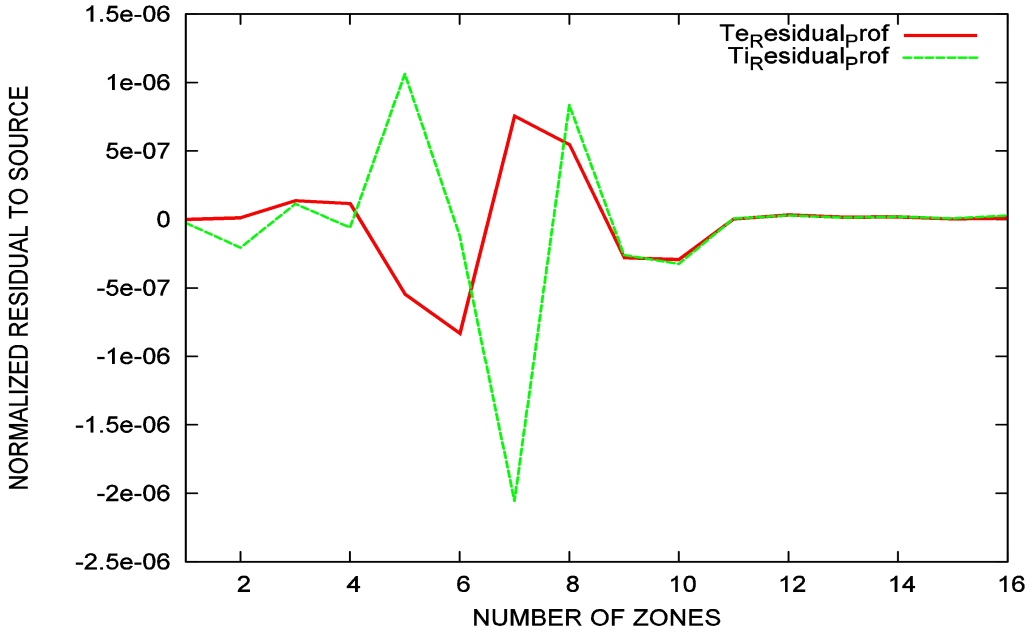
Test case

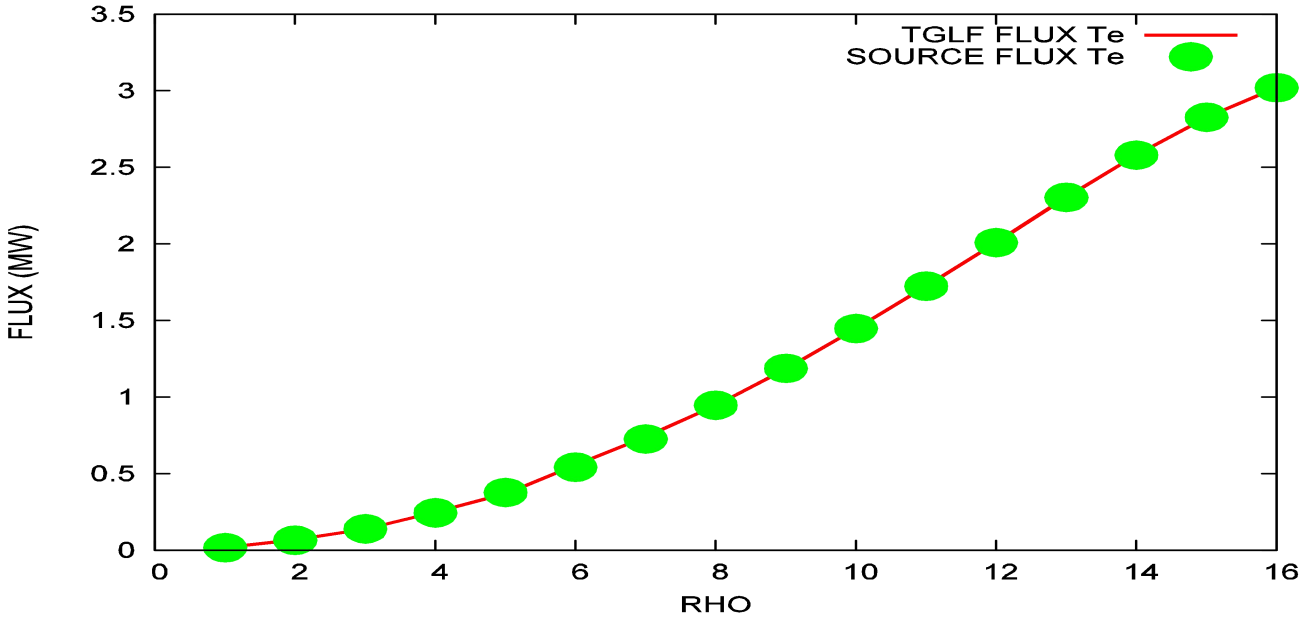
1): Reached steady-state solution after about 150 timesteps, each timestep requires several newton iterations to reach converged states. (dt=1.0d-3)

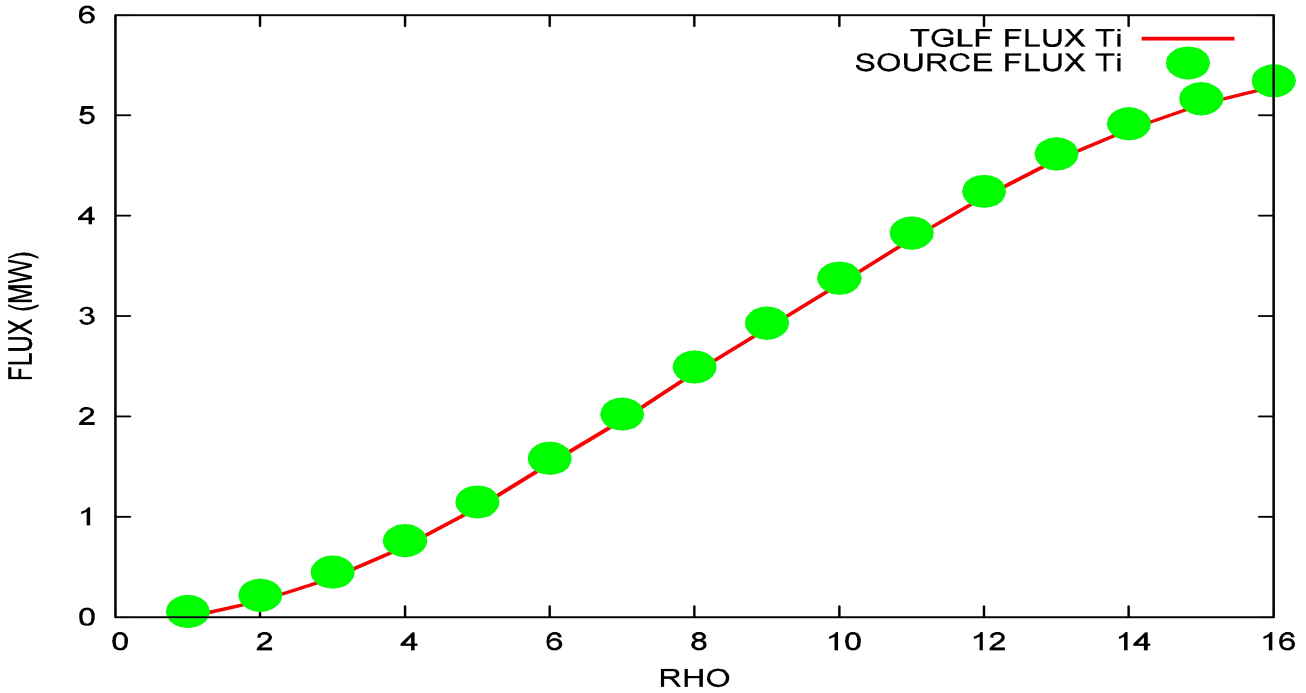
2): Normalized residual goes to level of 1.0e-6

3): Normalized residual profiles show good convergence close to boundary.









Test case

1): TGLF fluxes match the heat fluxes from the source terms (good convergence).

2): Many test runs show that IDO scheme is more robust than the existing algorithm that used in PT_SOLVER

3): This algorithm is not fast enough, it is still slow, however, it takes large timestep which will be good for steady-state phase of the job.

Summaries and discussions

Impurity density prediction capability is available for beta tester
1) : predict the radiation power loss
2): predict the individual impurity density profiles

IDO scheme is implemented as an alternative option in PT_SOLVER
1): fast for steady-state solution with large time step
2): still not fast enough for time dependent prediction using TRANSP PT_SOLVER
3): deep learning algorithm provides an encouraging methods to speedup
PT_SOLVER by factor of 10 to 100

the end